(19) World Intellectual Property Organization International Bureau



. | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| | 1001|| |

(43) International Publication Date 19 May 2005 (19.05.2005)

PCT

(10) International Publication Number WO 2005/045726 A2

(51) International Patent Classification7:

G06F 17/60

(21) International Application Number:

PCT/US2004/035444

(22) International Filing Date: 27 October 2004 (27.10.2004)

(25) Filing Language:

English

(26) Publication Language:

English

(30) Priority Data:

60/514,523 60/546,976 27 October 2003 (27.10.2003) U: 24 February 2004 (24.02.2004) U:

(71) Applicant (for all designated States except US): SSCI, INC. [US/US]; 3065 Kent Avenue, W. Lafayette, Indiana 47906 (US).

(72) Inventors; and

- (75) Inventors/Applicants (for US only): BATES, Simon [US/US]; 3343 Peppermill Drive, West Lafayette, Indiana 47906 (US). IVANISEVIC, Igor [US/US]; 331 Secretariat Circle, West Lafayette, IN 47906 (US). STAHLY, Barbara C. [US/US]; 3908 Sunnycroft Place, West Lafayette, Indiana 47906 (US).
- (74) Agents: GARRETT, Arthur S. et al.; Finnegan, Henderson, Farabow Garrett & Dunner, LLP, 901 New York Avenue, NW, Washington, D.C. 20001-4413 (US).

- (81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.
- (84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

 without international search report and to be republished upon receipt of that report

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: METHOD FOR INDEXING CRYSTALLINE SOLID FORMS

(57) Abstract: Crystalline solid forms may be characterized by their unit cell parameters through a process known as indexing. An embodiment of the invention scarches for the unit cell parameters of a crystalline solid form using a Monte-Carlo algorithm that incorporates certain rules to reduce search space. Another embodiment refines the results of the search to identify the correct unit cell parameters of the crystalline solid form. These methods may be automated, conveniently requiring little interaction from the user. The indexing method of the invention may be applied, for example, to distinguish between different crystalline solid forms of a substance.

